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Tool for Generation of MAC/GMC Representative Unit Cell for CMC/PMC Analysis

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September 2016

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Summary

This document describes a recently developed analysis tool that enhances the resident capabilities of the Micromechanics Analysis Code with the Generalized Method of Cells (MAC/GMC) 4.0. This tool is especially useful in analyzing ceramic matrix composites (CMCs), where higher fidelity with improved accuracy of local response is needed. The tool, however, can be used for analyzing polymer matrix composites (PMCs) as well. MAC/GMC 4.0 is a composite material and laminate analysis software developed at NASA Glenn Research Center. The software package has been built around the concept of the generalized method of cells (GMC). The computer code is developed with a user friendly framework, along with a library of local inelastic, damage, and failure models. Further, application of simulated thermomechanical loading, generation of output results, and selection of architectures to represent the composite material have been automated to increase the user friendliness, as well as to make it more robust in terms of input preparation and code execution. Finally, classical lamination theory has been implemented within the software, wherein GMC is used to model the composite material response of each ply. Thus, the full range of GMC composite material capabilities is available for analysis of arbitrary laminate configurations as well.

The primary focus of the current effort is to provide a graphical user interface (GUI) capability that generates a number of different user-defined repeating unit cells (RUCs). In addition, the code has provisions for generation of a MAC/GMC-compatible input text file that can be merged with any MAC/GMC input file tailored to analyze composite materials. Although the primary intention was to address the three different constituents and phases that are usually present in CMCs—namely, fibers, matrix, and interphase—it can be easily modified to address two-phase polymer matrix composite (PMC) materials where an interphase is absent. Currently, the tool capability includes generation of RUCs for square packing, hexagonal packing, and random fiber packing as well as RUCs based on actual composite micrographs. All these options have the fibers modeled as having a circular cross-sectional area. In addition, a simplified version of RUC is provided where the fibers are treated as having a square cross section and are distributed randomly. This RUC facilitates a speedy analysis using the higher fidelity version of GMC known as HFGMC. The first four mentioned options above support uniform subcell discretization. The last one has variable subcell sizes due to the primary intention of keeping the RUC size to a minimum to gain the speed ups using the higher fidelity version of MAC. The code is implemented within the MATLAB (The Mathworks, Inc., Natick, MA) developmental framework; however, a standalone application that does not need a priori MATLAB installation is also created with the aid of the MATLAB compiler.

Nomenclature

CovF; CovF	spread between the minimum and maximum fiber diameter
CovI; CovI	spread between the minimum and maximum interface outer diameter
d	dimension of square of same area as circular fiber with diameter d_f
d_c	distance from center of subcell to center of repeating unit cell (RUC)
d_f; Fdia	fiber diameter

$d_{f\,\max}$	maximum fiber diameter
$d_{f\,\min}$	minimum fiber diameter
Eclr; Eclr	fraction of fiber diameter from which the fiber clearance is calculated
k_f; FVR	fiber volume ratio
k_i; IVR	interface volume ratio
k_m	matrix volume ratio
L,*H*; L,H	length and height of RUC, respectively
N_f; $\mathrm{N_f}$	number of fibers in RUC
N_h	number of subcells along height of RUC
N_i; Ni	number of elements within interface
Npix; Npix	number of pixels along width or height of RUC
Nrep	number of RUCs for tiling
N_w	number of subcells along width of RUC
$\mathrm{N_x}$	number of subcells in x_2-direction of RUC
$\mathrm{N_y}$	number of subcells in x_3-direction of RUC
n_f	number of fiber subcells
n_i	number of interface subcells
R_f	radius of fiber
R_i	outer radius of interface
RadF	number of subcells used to define radius of fiber
RadI	number of subcells used to define radius of fiber plus interface
t_i	interface thickness
$t_{i\,\max}$	maximum interface thickness
$t_{i\,\min}$	minimum interface thickness
VarI	Boolean to indicate whether the thickness of interface is constant
VarP	fraction of interface thickness indicating the maximum variability of interface thickness
x_2, x_3	position of subcell
$x_2^{\text{new}}, x_3^{\text{new}}$	new position of mirrored subcell
x_i, y_i	fiber coordinates
ε	interfiber clearance distance

Introduction

The Micromechanics Analysis of Code with the Generalized Method of Cells (MAC/GMC) is an in-house-developed computer code. It can perform a comprehensive composite material and laminate analysis and is based on the generalized method of cells (GMC) micromechanics theory (Ref. 1). This theory enables access to the local stress and strain fields in the composite material that are crucial for assessing damage initiation and progression in composite structures. The software package has been built around GMC to provide a user friendly framework, along with a library of local inelastic, damage, and failure models. Further, application of simulated thermomechanical loading, generation of output results, and selection of repeating unit cell (RUC) architectures to represent the composite material have been automated in MAC/GMC 4.0. Finally, classical lamination theory has been implemented within MAC/GMC 4.0, wherein GMC is used to model the composite material response of each ply. Thus, the full range of GMC composite material capabilities is available for analysis of arbitrary laminate configurations as well. The many features that are available in the code as well as the procedures to

actually setup and run a problem are well described in the MAC/GMC 4.0 User's Manual—Example Problem Manual (Ref. 2) and the MAC/GMC 4.0 User's Manual—Keywords Manual (Ref. 3).

Preprocessing and postprocessing operations of MAC manually can be tedious, time consuming, and sometimes error prone. In order to facilitate these routine operations it is desirable to have dedicated software tools. Such tools currently exist for some aspects of MAC output postprocessing. Postprocessing of local stress and strain fields (MACPOST) of MAC are documented well in Reference 4. This program provided a link between MAC output files and MSC/PATRAN (Ref. 5). PATRAN was utilized to plot the local stress and/or strain contours, and stress-strain behavior. The current work, however, focuses primarily on the preprocessing aspects; specifically, the generation of a variety of RUCs suitable for analysis based on the theory of GMC. Current MAC/GMC capabilities do include a library of specialized representative unit cells for analysis of polymer matrix composites (PMCs) and ceramic matrix composites (CMCs). Typically PMCs have two constituents; fiber and matrix, and CMCs have three constituents; fiber, matrix, and interface. These RUCs can be accessed on the fly during the analysis. Also, there are provisions for user-defined RUCs. For details of the available RUCs the reader may refer to Reference 2. The resident RUC capabilities, however, are often limited for advanced analyses where higher fidelity of the local response, and a detailed representation of the microstructure variability are needed. For example, Figure 1 shows a micrograph of a typical CMC material consisting of fiber, matrix, interface, and voids. The fibers have different diameters. Furthermore, the interface thicknesses varies along the circumference of the fiber. In addition fibers are distributed randomly within the material.

User-defined RUCs sometimes involve extensive tailoring in order to satisfy one's requirements. For example, if one has to represent accurately a micrograph in order to capture the stochastic nature of the microarchitecture, the procedure becomes extremely tedious and time consuming without an automated procedure. Not to mention, input errors become more likely with manual intervention. Keeping this in mind, a project has been undertaken to generate RUCs routinely without requiring the user's manual intervention and thus speedup the MAC/GMC input generation process. What follows herein is a description of the in-house RUC generator software package with a graphical user interface (GUI) and its usage.

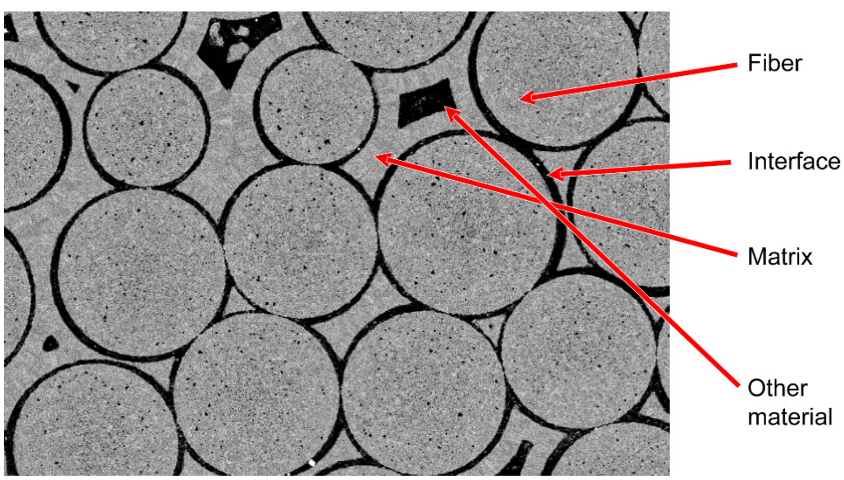

Figure 1.—Typical micrograph of ceramic matrix composite (CMC) material showing variability in fiber diameter, interface thickness, voids, and other free particles.

Design of the GUI

Figure 2 shows the design details of the user interface. Shown at the top are five main options the user may select. Each one pertains to a type of RUC. The design of the GUI follows context-sensitive windows, tables, and buttons such that depending upon the user choice, only the appropriate windows and buttons are shown, and all the other details are suppressed. This keeps a clean and uncluttered look to the interface. The next few paragraphs detail every option and show the appropriate input boxes that the user needs to fill in depending the requirements.

HexFvr

As the name suggests, this option invokes the generation of an RUC suitable for hexagonal packing of fibers. The fiber is circular shaped. When a user selects the “radio” button for HexFvr, the GUI looks like Figure 3. As indicated, the user is required to provide four parameters. Each parameter is described below:

1. Ni: Approximate number of subcells to represent the thickness of interface radially. The user normally selects 1. The default value is also set as 1. However, if a highly dense mesh is desired higher number for Ni may be specified. The size of the RUC depends on Ni.
2. FVR: Fiber volume ratio
3. IVR: Interface volume ratio
4. Nrep: Number of repetitions to tile the RUC in both x- and y-directions

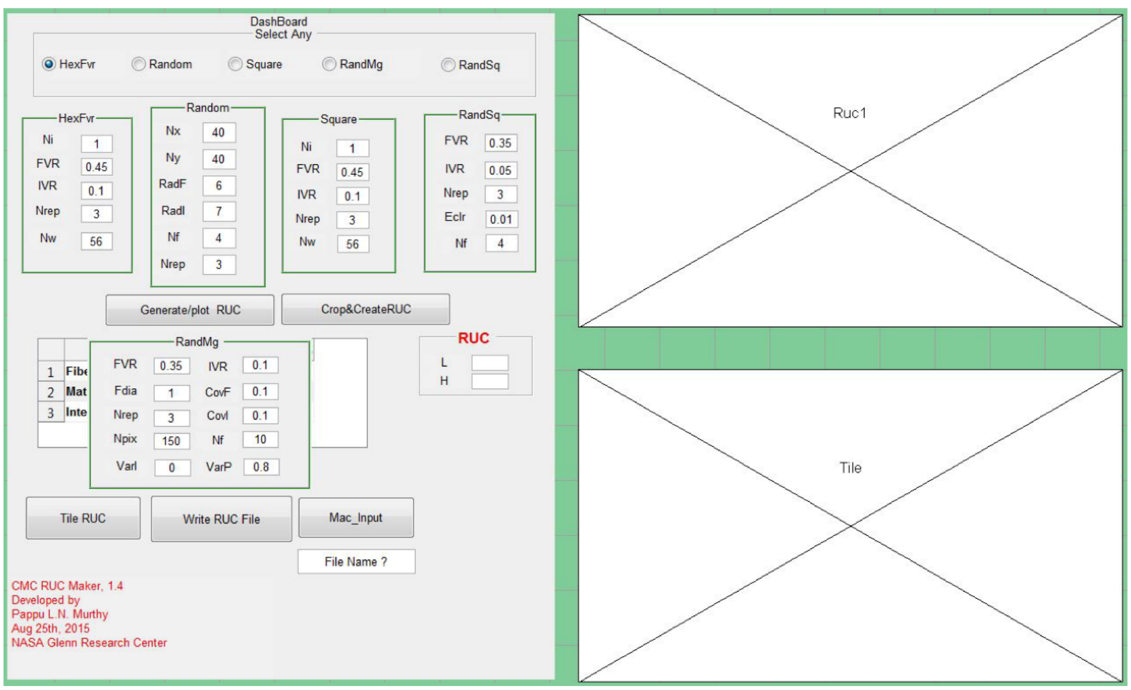

Figure 2.—CMC repeating unit cell (RUC) Generator Interface Layout.

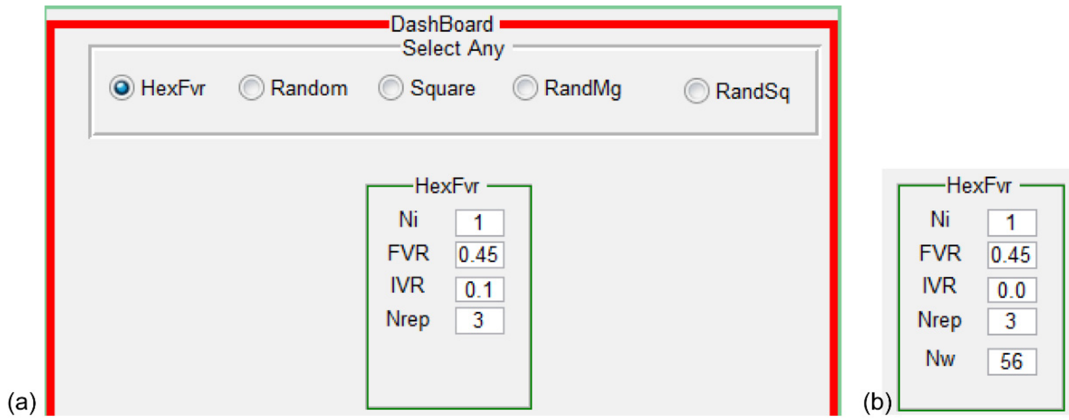

Figure 3.—User options for hexagonally packed CMC and polymer matrix composite (PMC) RUCs. (a) CMC RUC. (b) PMC RUC. User chooses IVR = 0.

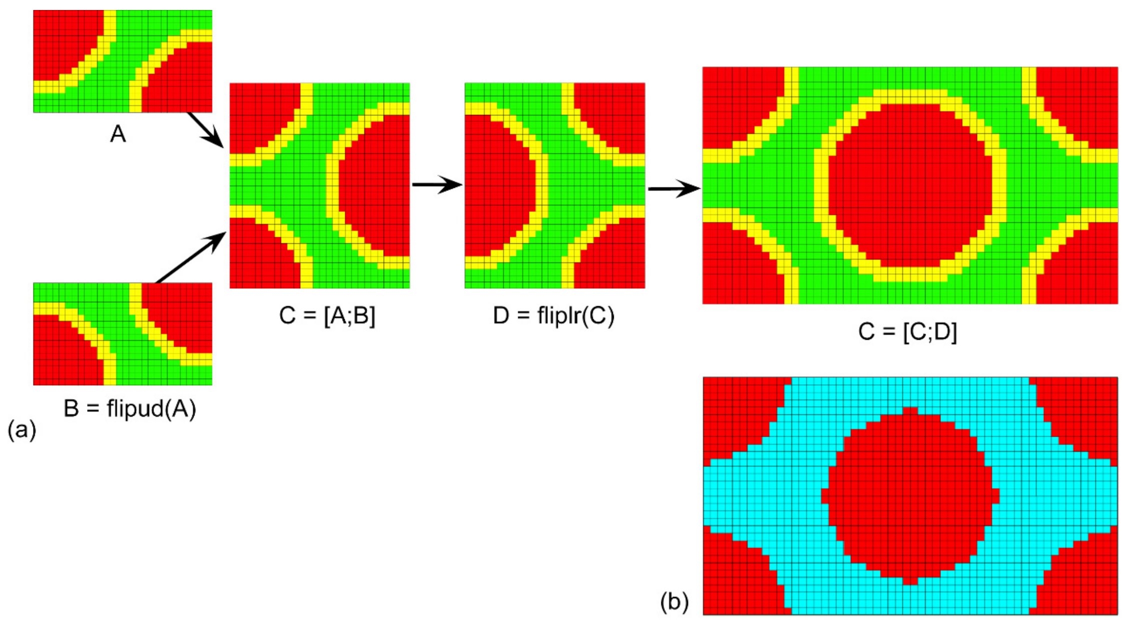

Figure 4.—Progression of subcell generation for a hexagonally packed RUC. (a) CMC RUC. (b) PMC RUC.

Based upon the above provided information, the program generates an RUC, shown in Figure 4. The basic building block for the RUC is segment A, which is generated based on the four parameters mentioned above. The height of RUC is determined based on the width, by using the formula height = 0.866×width, which is then rounded to the nearest integer. The height and width of the RUC are chosen based on FVR and IVR. As shown in Figure 4, segment B of the RUC is generated next, by flipping the image shown in segment A upside down. A and B are then combined as shown in C. Segment D is formed next by flipping image C left to right as shown. Segments C and D are then combined to arrive at the final version of the RUC shown in E. The program tries to iterate as much as possible by varying the thicknesses of the interface and the fiber radius to match the desired FVR and IVR as closely as possible. However, it should be kept in mind this is not always possible because the code utilizes a uniform grid discretization. The intention of the details given here, that may look trivial, is to aid users wishing to develop code for other types of packing such as diamond and rhombus. The above steps are still applicable with slight modifications to achieve the desired result. The last parameter Nrep is utilized to build a tiled version of the RUC. The RUC is repeated Nrep×Nrep times in both directions resulting in Nrep×Nrep fibers. Results are shown when user selects the button “Tile Ruc” for tiling.

Users wishing to develop an RUC for a PMC material with no interface need to specify IVR = 0. A new box appears as shown in Figure 3(b) where the user specifies the number of subcells in the width direction. Generation of the PMC RUC follows essentially the same steps as outlined above.

Generation of the RUC starts once the user completes all the information in the various boxes and then chooses the button “Generate/plot RUC.” Figure 5 shows the results. The details include the actual fiber, matrix, and interface volume ratios realized as well as the dimensions of the final RUC. Additionally, the buttons “Tile Ruc” and “Mac_Input” appear. The “Mac_Input” button, when selected, creates a text file consisting of the *RUC input block for MAC/GMC input. Readers wishing to know the details of the MAC/GMC input file may refer to the MAC/GMC user manual (Ref. 2). Figure 6 shows the results of the complete execution for a PMC hexagonally packed RUC.

Context-sensitive helpful hints are provided for all of the text boxes and the buttons. So a user who wants to know more about a particular box or a parameter can hover the mouse pointer over the object to see a short description of a helpful hint for that particular object.

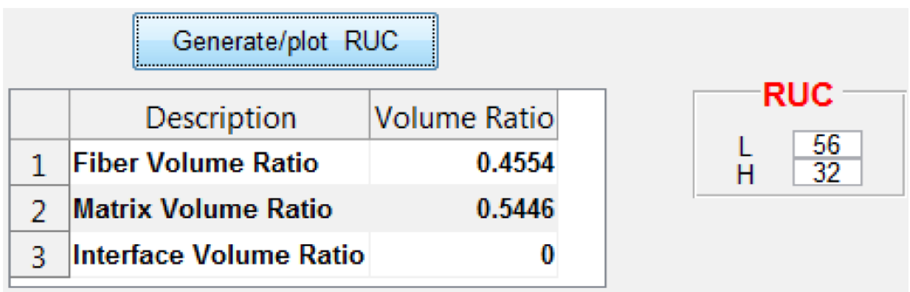

Figure 5.—Details of RUC that appear once user chooses to “Generate/plot RUC.”

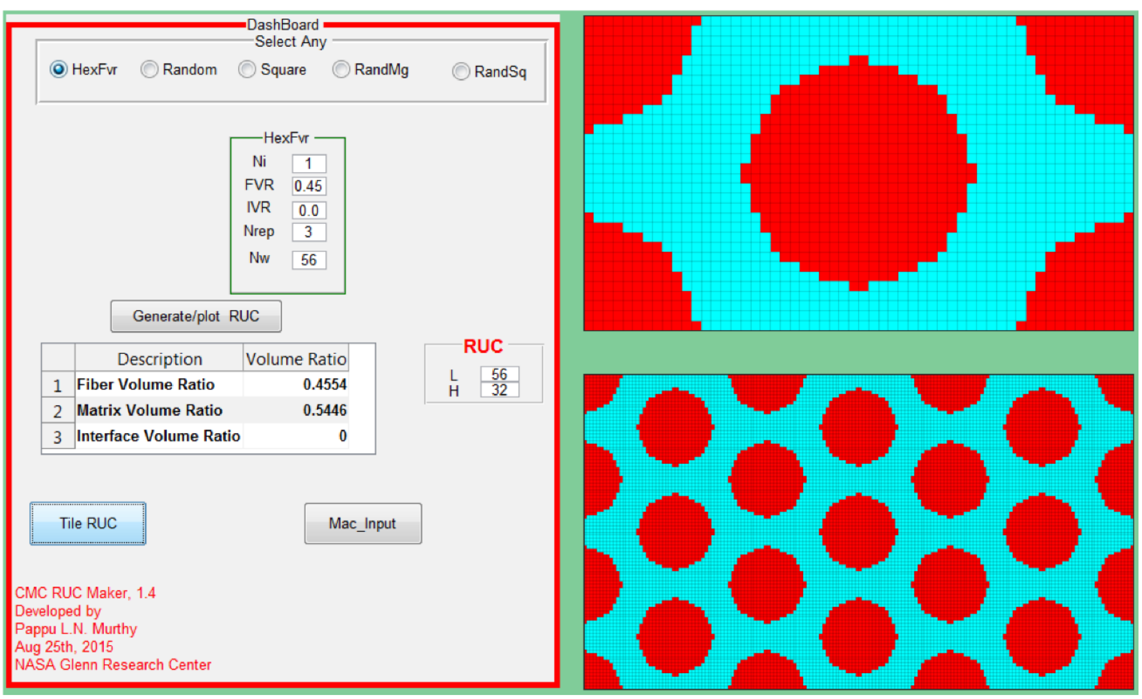

Figure 6.—Graphical user interface (GUI) generation of hexagonally packed RUC representation for PMC.

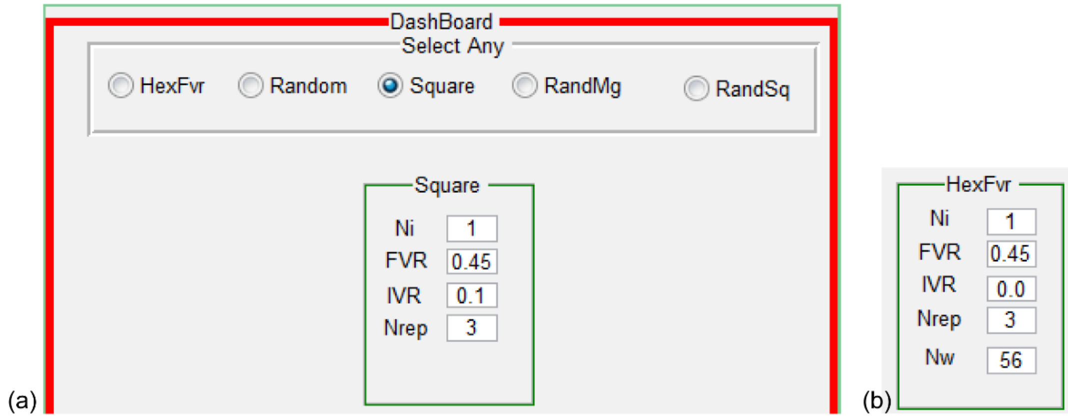

Figure 7.—User options for square-packed CMC and PMC RUCs. (a) CMC RUC. (b) PMC RUC. User chooses IVR = 0.

Square

This option is chosen when a simple square packing with a circular fiber is desired in an RUC. The input parameters are shown in Figure 7(a). As indicated, the user is required to provide four parameters. Each parameter is described below:

1. Ni: Number of subcells for interface. The user normally selects 1. The default value is also set as 1. However, if a highly dense mesh is desired a higher number for Ni may be specified. The size of RUC depends on Ni.
2. FVR: Fiber volume ratio, k_f
3. IVR: Interface volume ratio, k_i
4. Nrep: Number of repetitions to tile the RUC

Notice that the parameters are the same as the ones for HexFvr case. However, the subcell generation scheme is entirely different. Based on the FVR and IVR, the initial fiber radius and interface thickness are determined using the following equations:

$$R_f = \sqrt{\frac{k_f}{\pi}} \qquad R_i = \sqrt{\frac{k_f + k_i}{\pi}} \qquad t_i = R_i - R_f \tag{1}$$

where R_f and R_i are the fiber and interface outer radii, respectively, and t_i is the interface thickness. Further, the RUC is assumed to be a square of 1 unit. Based on N_i and t_i, the number of subcells along the width and height (N_w and N_h, respectively) are determined using

$$N_w = N_h = \mathrm{round}\left(\frac{N_i}{t_i}\right) \tag{2}$$

If the equation returns an odd number, it is converted to an even number by subtracting 1.

For square-packed RUCs, the number of subcells along the width and height are the same ($N_h = N_w$). Next, the subcells are assigned a material identification number 1 for fiber, 2 for matrix, and 3 for the interface. The material is determined using the following code:

$$\begin{array}{l} \text{if} \\ d_c \leq R_f \\ \text{material is 1 (fiber)} \\ d_c > R_f \text{ and } d_c \leq R_i \\ \text{then material is 3 (interface)} \\ \text{else} \\ \text{material is 2 (matrix)} \\ \text{end} \end{array} \tag{3}$$

In the above, d_c is the distance from the center of a subcell to the center of the RUC. The above logic may not always give exact values for the FVR and IVR because of the uniform discretization. In order to improve the accuracy the radius of the fiber and interface are varied slightly for the best possible result.

Users wishing to develop an RUC for a PMC material with no interface need to specify IVR = 0. A new box appears as shown in Figure 7(b) where user specifies number of subcells in the width direction. Generation of the PMC RUC then follows essentially the same steps as outlined above.

The buttons “Generate/plot RUC,” “Tile RUC,” and “Mac_Input” function just as described in the previous section. Figure 8 shows the final results for a square-packed RUC.

Random

This option if selected invokes random placement of circular fibers within the RUC domain and can be used to generate RUCs that more closely resemble the actual microstructure of the CMC/PMC. When the user selects the “radio” button for Random, the GUI looks like Figure 9. As indicated, the user is required to provide six parameters. Each parameter is described below.

1. N_x: Number of subcells in the x_2-direction of the RUC. Used to define total size of RUC
2. N_y: Number of subcells in the x_3-direction of the RUC. Used to define total size of RUC
3. RadF: Number of subcells used to define the radius of the fiber
4. RadI: Number of subcells used to define the radius of the fiber plus the interface
5. N_f: Number of fibers to be placed in the RUC
6. Nrep: Number of repetitions to tile the RUC

Users wishing to develop RUCs for PMC materials with no interface need to specify RadI = RadF.

It should be noted that the default values provided in various boxes are meant to guide the user; however, the user needs to experiment with different values until the desired requirements are met. Based upon the above provided information, the program generates an RUC as shown in Figure 9. The basic building block for the random-packed RUC is a square RUC similar to that shown in Figure 8. This building block RUC (BBRUC) is created using the RadF and RadI information provided by the user. A random number generator is used to select the center position for the fiber, and the BBRUC is placed in the RUC, which is initially composed of only matrix subcells, such that the center of the BBRUC corresponds to this randomly generated position.

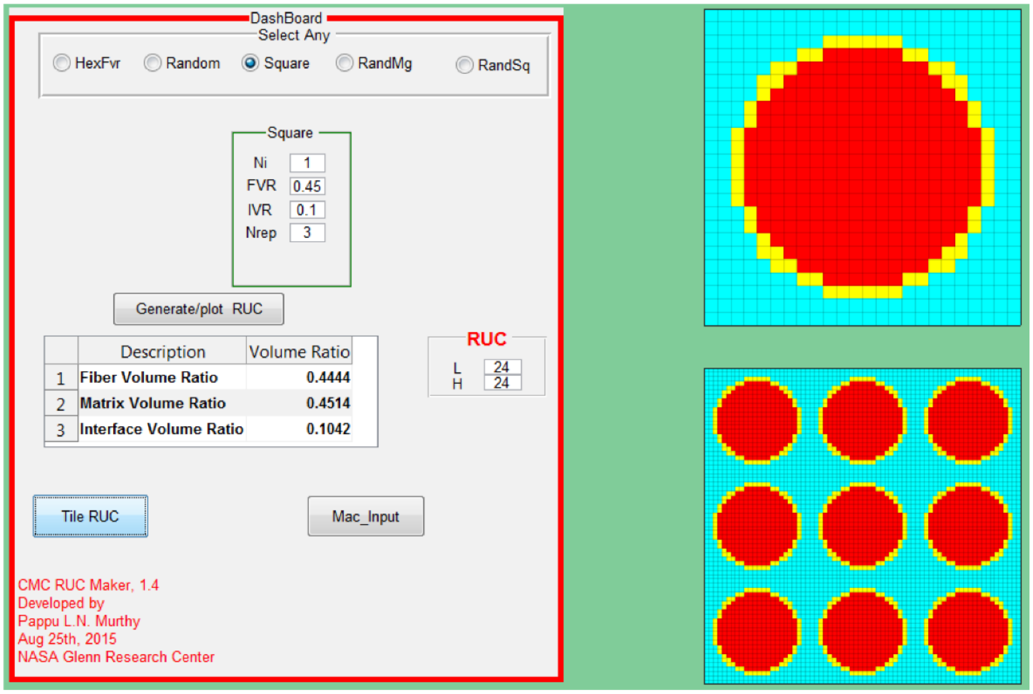

Figure 8.—GUI generation of square-packed RUC representation for CMC.

Since the center position of the BBRUC is random, the position of the center of the fiber may be chosen such that the boundaries of the fiber or interface lie beyond the boundaries of the RUC. In these cases, the subcells that would fall outside of the RUC boundaries are reflected, or mirrored, across the appropriate RUC boundaries.

$$
\begin{aligned}
x_2^{\text{new}} &= x_2 - N_w \text{ (or } N_x\text{); if } x_2 > N_w \text{ (or } N_x\text{)} \\
x_2^{\text{new}} &= x_2 + N_w \text{ (or } N_x\text{); if } x_2 < 1 \\
x_3^{\text{new}} &= x_3 - N_h \text{ (or } N_y\text{); if } x_3 > N_h \text{ (or } N_y\text{)} \\
x_3^{\text{new}} &= x_3 + N_h \text{ (or } N_y\text{); if } x_3 < 1
\end{aligned}
\tag{4}
$$

Following Equation (4), the original position of the subcell $[x_2, x_3]$ is moved to $[x_2^{\text{new}}, x_3^{\text{new}}]$. Prior to placing the BBRUC, the code checks two conditions:

1. None of the fiber or interface subcells can be placed in locations already occupied by a fiber or interface subcell of a previously placed BBRUC.
2. At least one matrix subcell must be present between any fiber and/or interface subcells in the current BBRUC and those belong to previously placed BBRUCs.

If either of these conditions are violated, a new random number is generated for the fiber center, and the conditions are checked again. This procedure iterates until both conditions are satisfied, and a suitable position for the BBRUC in the RUC is found. For large FVR, the RUC instance may not contain any locations for the current BBRUC that still satisfies the two constraints. Thus, a new RUC instance will be created after a maximum number of iterations is exceeded.

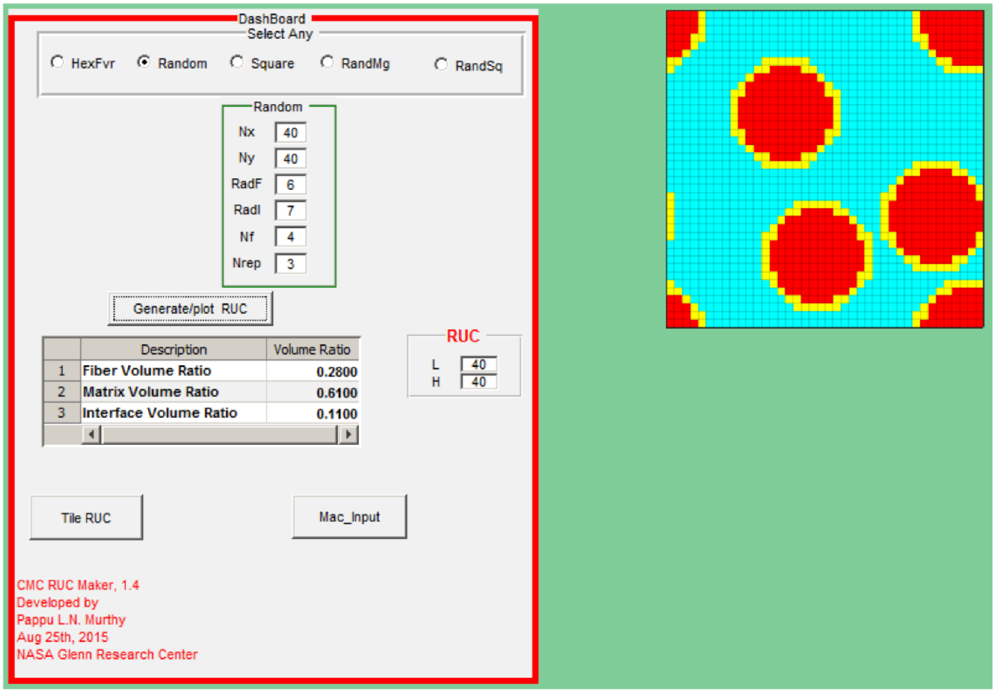

Figure 9.—GUI generation of randomly packed RUC representation for CMC.

Figure 9 shows the results after choosing the button "Generate/plot RUC," and the complete execution for a CMC random packing RUC is concluded. Unlike the other RUC-generation techniques, the actual fiber, interface, and matrix volume ratios (k_f, k_i, and k_m, respectively) realized are outputs of the Random procedure and are calculated accordingly:

$$k_f = \frac{n_f}{N_w N_h} \tag{5}$$

$$k_i = \frac{n_i}{N_w N_h} \tag{6}$$

$$k_m = 1 - k_f - k_i \tag{7}$$

RandMg

When the user wants to develop a highly detailed RUC from actual composite micrographs the "RandMg" option may be utilized. The input parameters are shown in Figure 10. As indicated, the user is required to provide 10 parameters. Each parameter is described below.

1. FVR — Fiber volume ratio, k_f
2. IVR — Interface volume ratio, k_i
3. Fdia — Fiber diameter
4. CovF — Difference between minimum and maximum diameters of the fiber, user chooses 0 if no variability of fiber diameter is desired
5. Nrep — Number of repetitions for tiling purpose
6. CovI — Difference between minimum and maximum outer diameters of the interface. User choses 0 if no variability of interface thickness is desired.

7. Npix Number of pixels in width and height of RUC
8. Nf Number of fibers in RUC
9. VarI A true or false flag that informs the program whether the interface is concentrically located such that the thickness is constant (0), or not, such that the thickness varies circumferentially (1).
10. VarP If variable thickness is desired then this parameter defines the fractional amount of interface thickness by which the center is to be perturbed so as to generate a variable thickness interface that is normal to a typical micrograph (Fig. 1).

As shown in Figure 10, default values are provided for all parameters, which may be overridden by the user depending on the requirements. Most of these parameters need to be determined a priori by performing a thorough image analysis of composite micrographs. The defaults shown here are only for guidance and are just typical values for a CMC material.

What follows in the next few paragraphs is a brief description of the theoretical consideration in the generation of the RUC. The process starts by establishing the dimensions of the RUC based on the average diameter, d_f (Fdia), number of fibers N_f (Nf), and the fiber volume ratio k_f (FVR), using the following equation:

$$L = H = \sqrt{\left(\frac{N_f \pi d_f^{\,2}}{4k_f}\right)} \tag{8}$$

It should be noted that the derivation is quite straightforward and therefore details are not shown. The quantity under the square root is the total cross-sectional area of all the fibers divided by the fiber volume ratio, which leads to the area of the RUC (L×H).

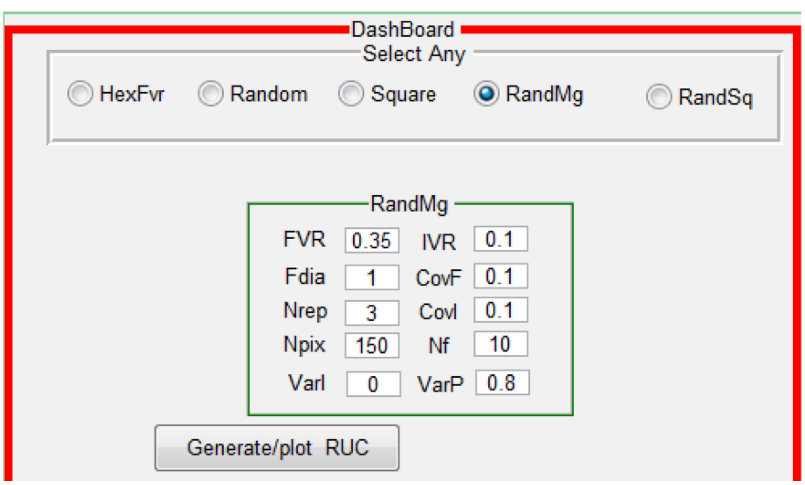

Figure 10.—User selects “RandMg.” Shown are parameters and their default values, which may be overwritten by user to meet requirements.

The average interface thickness is next calculated using the following equation:

$$t_i = \sqrt{\frac{\left(\frac{N_f \pi d_f^{\,2}}{4} + LHk_i\right)}{\pi N_f}} - \frac{d_f}{2} \tag{9}$$

Based upon the user's choices for the differences between the minimum and maximum fiber diameters and interface outer diameter, the limits for fiber and interface outer diameters are established next.

$$\begin{aligned} d_{f\,\mathrm{min}} &= \left(\frac{1 - CovF}{2}\right) d_f \\ d_{f\,\mathrm{max}} &= \left(\frac{1 + CovF}{2}\right) d_f \\ t_{i\,\mathrm{min}} &= \left(\frac{1 - CovF}{2}\right) t_i \\ t_{i\,\mathrm{max}} &= \left(\frac{1 + CovI}{2}\right) t_i \end{aligned} \tag{10}$$

The next phase of RUC generation involves randomly generating fibers and the outer diameter of interface with diameters distributed according to a beta random distribution between the limits shown in Equation (10). Fibers are generated one at a time with the corresponding interface and randomly placed within the square domain defined by the *L* and *W* dimensions. The centers of the fibers are generated by a uniform distribution defined within the RUC domain. Once a fiber position is generated and placed within the RUC domain, it is then checked to see whether it is completely inside the domain or intersecting any of the boundaries $x = 0$ or L, and $y = 0$ or H. If the fiber intersects a boundary then the remaining portion of the fiber is copied to the opposite side by generating identical fiber, but with centers $(x \pm L, y \pm H)$. This is illustrated in Figure 11(a). In this specific case, the randomly generated fiber center (x_i, y_i) happens to intersect the right-side boundary. So the remaining portion of the fiber is mirrored to the left side by placing a fiber at center $(x_i - L, y_i)$. Extending this logic, suppose the fiber were to intersect the boundaries at one of the corners, for example the top right-hand corner. In this case, portions of the fiber have to be placed in all three corners using the centers $(x_i - L, y_i)$ for the top left corner, $(x_i - L, y_i - H)$ for the bottom left corner, and $(x_i, y_i - H)$ for the bottom right corner. Notice that such logic is necessary in order to preserve the periodicity boundary conditions for the RUC, which is central to the GMC theory.

Once a fiber is placed, a second fiber center is generated randomly within the RUC domain. Now, a check has to be made to see whether this fiber position is feasible. It is only possible by meeting the following conditions:

1. It shall not intersect any other fiber that is already successfully placed within the domain.
2. If the fiber intersects any boundary, the corresponding opposite boundary must have a vacant place to fill the remaining portion of the fiber.

Once the above two conditions are satisfied, then it is feasible to place the second fiber. If any of the above conditions are violated, then the center point is rejected, a new center is randomly generated, and the process moves on.

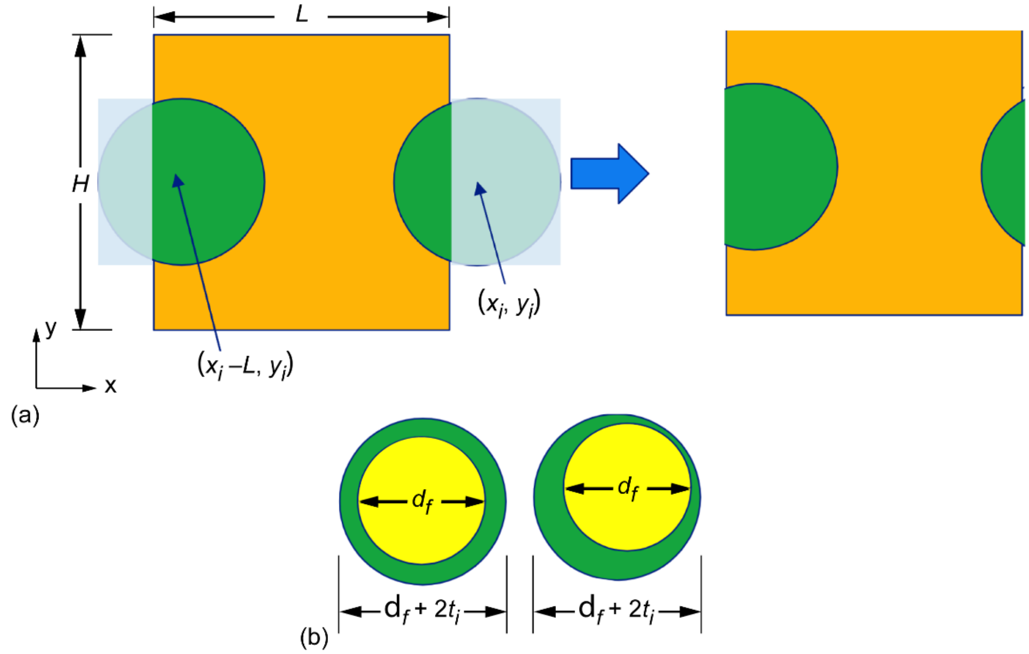

Figure 11.—Random placement of fiber that is intersecting one of the boundaries (right side boundary in this case). This is necessary to maintain periodic boundary condition for RUC. (a) Mirroring remaining portion of fiber to left side by placing fiber at center ($x_i - L$, y_i). (b) Placing fiber either concentrically or eccentrically, depending on user choices for variability of interface thickness.

The above process continues until all of the fibers are successfully placed within the RUC, and they satisfy the periodic boundary conditions as well as the requirement that the fibers do not intersect each other. At this point, the generation of the RUC is complete except for the subcell discretization. It should be noted here that the diameters of the fibers shown include the interface. The actual fiber is placed concentrically inside the outer diameter formed by interface as shown in Figure 11(b). Once the generation of all fibers is successfully completed, the program checks for interface thickness variability, VarI. If VarI is 1, then the parameter VarP is used to generate a small eccentricity around the fiber center, resulting in a somewhat eccentrically located fiber, which yields a variable-thickness interface.

Generation of the RUC starts once the user completes all the information in the various boxes by choosing the button “Generate/plot RUC.” Figure 12 shows the results. In this specific example there are 10 fibers with varying fiber diameters and interface thicknesses. Extreme values for CovF (0.3) and CovI (0.3) were chosen so that the variability in the microstructure can clearly be seen in Figure 13. It should be noted that several fibers are cut off at the boundaries, but since the program enforces periodicity when tiled, the RUC will have whole fibers everywhere.

Actual generation of the subcells within the RUC starts next in the sequence of operations. The user-specified value of Npix (number of pixels along the x- and y-directions) is used to discretize the RUC into Npix-by-Npix subcells. Each subcell is subsequently assigned a value of 1 for fiber, 2 for matrix, and 3 for interface depending on where the center of each subcell lies within the RUC region. This process is started by using the button “CropandCreateRUC.” Results are shown in Figure 13. The actual FVR and IVR that are realized for the given uniform discretization are also shown. As mentioned earlier, because of uniform discretization it is not possible to satisfy the exact FVR and IVR requirements. Increasing the number of pixels for the RUC will improve the accuracy. At the end of the discretization operation, the buttons “Tile Ruc” and “Mac_Input” appear to perform the finishing operations as mentioned previously.

The default values provided are based upon actual measured data from a typical micrograph. These values must be changed according to the composite material micrograph in investigation.

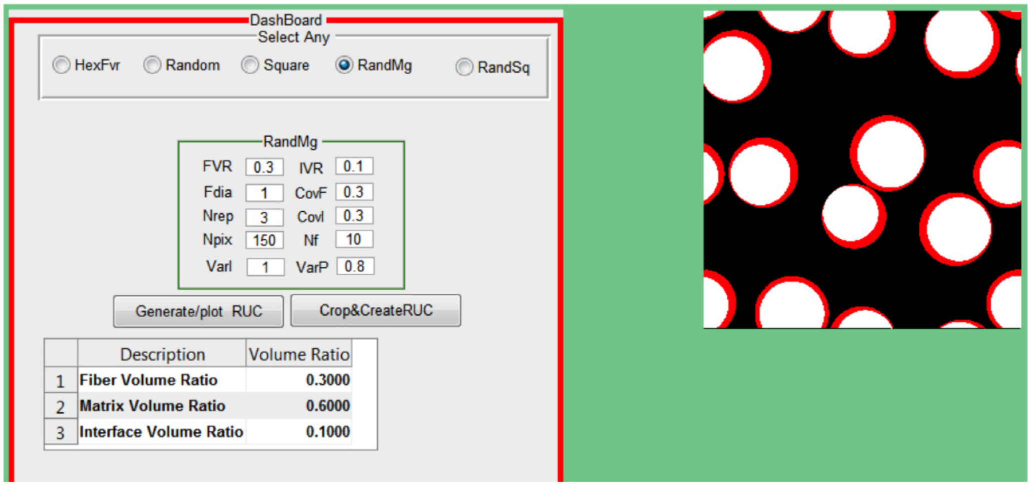

Figure 12.—Microstructure-based RUC generation.

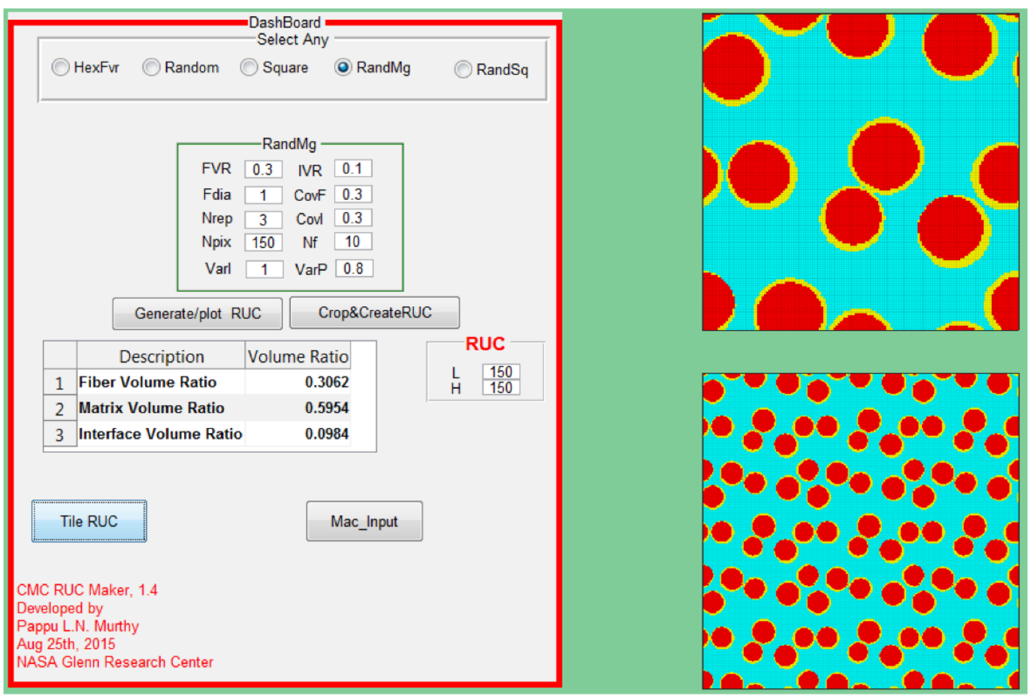

Figure 13.—A 150-by-150 RUC for CMC material. Also shown is 3-by-3 RUC tiling.

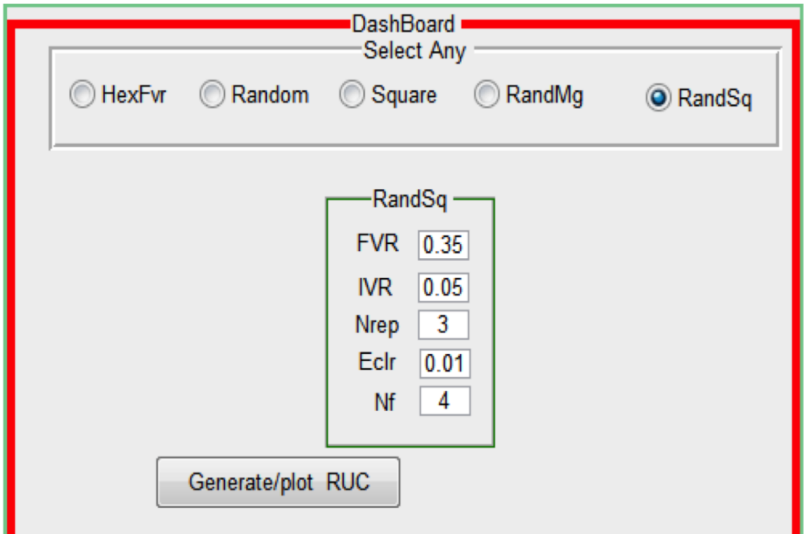

Figure 14.—Parameter inputs for "RandSq" choice.

RandSq

This option is provided to generate RUCs that have enough fidelity, yet run much faster than the micrograph-based RUCs generated using the "RandMg" option or the RUCs generated using the "Random" option described above. The main difference is that the fiber cross sections are treated as squares, and the discretization is not uniform. So one can achieve exact fiber and interface volume ratios by adjusting the sizes of the subcells, which are in general rectangular. Furthermore, the size of the RUC is much smaller compared to either of the two above-mentioned cases. The number of subcells in a typical fiber is much smaller compared to a uniform RUC discretization. However, the surrounding matrix is divided fine enough to capture the local damage events fairly accurately. The input parameters are shown in Figure 14. As indicated, the user is required to provide five parameters. Each parameter is described below.

1. FVR — Fiber volume ratio, k_f
2. IVR — Interface volume ratio, k_i
3. Nrep — Number of repetitions for tiling purpose
4. Eclr — Clearance between fibers in order to assure that fibers do no touch. Notice that this option was not needed for all other cases considered above since the discretization was uniform, and there was always at least one subcell of matrix between the fibers.
5. Nf — Number of fibers in RUC according to the user choice

As shown in Figure 14, default values are provided for all parameters. These values may be overridden by the user depending on requirements. The fiber dimensions are assumed to be a square of side d, and the dimensions of the RUC are determined by

$$L = H = \sqrt{\frac{d^2 N_f}{k_f}} \tag{11}$$

The thickness of the interface is calculated by using the equation

$$t_i = \left(\frac{\sqrt{\left(LHk_i + N_f d^2\right) / N_f} - d}{2} \right) \tag{12}$$

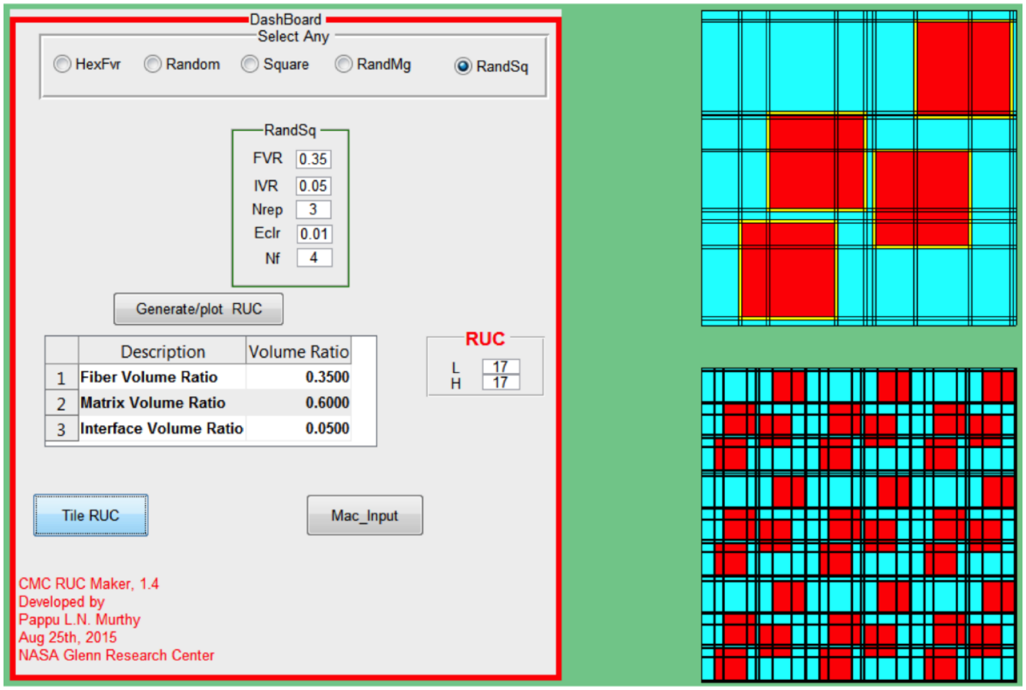

Figure 15.—Square fibers in square packing with nonuniform discretization.

Once the dimensions of RUC are established, a small clearance is added all around the fiber/interface combination, so that when these are generated and placed randomly within the RUC, they do not touch. This clearance value is calculated to be

$$\varepsilon = Eclr \times d_f \tag{13}$$

The random placement of fibers within the RUC region defined as L by H, follows the same procedure as that for the "RandMg" option described above. Once all the fibers are placed, the subcell grid is formed by drawing vertical and horizontal lines along the fiber boundaries and the interface boundaries. This would give the minimum possible number of subcells for a given RUC. If higher fidelity is desired, the subcells can further be discretized by dividing each subcell into 2×2 (four) subcells. Currently, this option does not support higher fidelity subdivisions. Further, all fibers are assumed to have the same dimensions and the interface thickness is assumed to be constant around the fiber located concentrically. Future versions of the code will relax these assumptions further.

As in all previous cases, the process of RUC generation starts when the user clicks on button "Generate/plot RUC." Results are shown in Figure 15. It should be noted that the realized FVR and IVR match exactly the user requirements in this case.

Recommendations

Several options for the generation of RUCs are presented above, and the question remains; what should one use? This largely depends on the specific application and desired accuracy that the user requires, and no single option fits all the cases. An appropriate RUC must be chosen according to the user's requirements. For example, when a user wants to compare the performance of GMC vs. HFGMC for a PMC/CMC with just one fiber, options HexFVr or Square are most appropriate, with or without IVR. Furthermore, if local damage needs to be investigated in detail, a sufficiently fine grid on the order of 30 to 60 subcells along one dimension may be needed. Such would be the case when fatigue, creep, or the nonlinear stress strain response of a composite are desired.

If the user wants to investigate the effect of slightly perturbed to randomly distributed fibers within the RUC, then the option “Random” is most appropriate. This option generates a fairly dense discretization (30×30 to 60×60) depending on the number of fibers and also assures that periodic boundary conditions are satisfied. This option is extremely useful when studying the effect of randomly perturbed microstructures on composite fatigue, creep, and strength response, as well as the statistics of effective properties of the composite due to microstructure variability.

Often, the user might want to investigate an actual micrograph much closer, by taking measurements of individual fibers, interface thicknesses, voids, and other practical nuances. In order to represent these practical situations, the option “RandMg” is extremely useful in capturing all the details in a fairly accurate manner. The resulting RUCs are usually of the order of 100s by 100s subcells.

Concluding Remarks

A fairly comprehensive treatment of the generation of composite repeating unit cells (RUCs) is presented herein. Enough details and guidelines are provided, so that the user can make an appropriate choice of RUC for a specific application. The tool enables the user to create the RUC input block of Micromechanics Analysis Code with the Generalized Method of Cells (MAC/GMC) code input file. The tool is based on a graphical user interface (GUI) concepts. All the buttons are accompanied with context sensitive helpful tips to guide the user.

References

1. Paley, M.; and Aboudi, J.: Micromechanical Analysis of Composites by the Generalized Cells Model. Mech. Mater., vol. 14, 1992, pp. 127–139.
2. Bednarcyk, Brett A.; and Arnold, Steven M.: MAC/GMC 4.0 User’s Manual—Keywords Manual. NASA/TM—2002-212077/VOL2, 2002. http://ntrs.nasa.gov
3. Bednarcyk, Brett A.; and Arnold, Steven M.: MAC/GMC 4.0 User’s Manual—Example Problem Manual. NASA/TM—2002-212077/VOL3, 2002. http://ntrs.nasa.gov
4. Goldberg, Robert K.; Comiskey, Michele D.; and Bednarcyk, Brett A.: Micromechanics Analysis Code Post-Processing (MACPOST) User Guide. Version 1.0, NASA/TM—1999-209062, 1999. http://ntrs.nasa.gov
5. MSC/PARAN User Manual, version 8.0. MacNeal-Schwendler Corporation, Los Angeles, CA, 1998.